Supporting Information for

Development of a unit-based industrial emission inventory in the Beijing-Tianjin-Hebei region and resulting improvement in air quality modeling

There are several studies estimating emissions in BTH region. We compare emissions reported after 2014 (the base year is 2010 or later) with our study, which are shown in **Fig.S3**.

For SO_2, NOx and $PM_{2.5}$, in Beijing, the total emissions in our study (for 2014) are significantly lower than those in previous studies (for 2010-2013), probably because stringent control measures have been implemented during 2010-2014. In Tianjin and Hebei, the emission estimates from different studies are much closer to each other. For NMVOCs, Wang et al. (2014), Wu et al. (2017) and Cai et al. (2017) generally have similar results to this study. The NMVOCs emissions by Zheng et al. (2017) are higher in Beijing and Tianjin, and lower in Hebei compared with other studies. For NH_3 emissions, the estimates from various studies are generally similar, except that the estimate of Zhou et al. (2015) is much higher.

We compare the meteorological parameters simulated by WRFv3.7 with observational data obtained from the National Climatic Data Center (NCDC), where hourly or 3-h observations are available for about 28 sites in the innermost domain. The variables of interest include the temperature at 2 m, wind speed at 10 m, and humidity at 2 m. The statistical indices used include the mean observation (Mean OBS), mean simulation (Mean SIM), mean bias, gross error, root mean square error (RMSE), and index of agreement (IOA), the definitions of which are provided in Emery et al. (2001). Table S1 summarizes the model performance statistics as well as the benchmarks suggested by Emery et al. (2001). Obviously almost all indices fall within the benchmark range except that the MB of humidity slightly exceeds the range in July. In summary, the statistics indicate an overall decent performance of meteorological predictions.

Reference:

Cai, S., Wang, Y., Zhao, B., Wang, S., Chang, X., and Hao, J.: The impact of the "Air Pollution Prevention and Control Action Plan" on PM2.5 concentrations in Jing-Jin-Ji region during 2012-2020, Sci Total Environ, 580, 197-209, 10.1016/j.scitotenv.2016.11.188, 2017.

Emery, C., Tai, E., and Yarwood, G.: Enhanced meteorological modeling and performance evaluation for two texas episodes, Report to the Texas Natural Resources Conservation Commission. (ENVIRON, International Corp, Novato, CA), 2001.

Wang, S. X., Zhao, B., Cai, S. Y., Klimont, Z., Nielsen, C. P., Morikawa, T., Woo, J. H., Kim, Y., Fu, X., Xu, J. Y., Hao, J. M., and He, K. B.: Emission trends and mitigation options for air pollutants in East Asia, Atmos Chem Phys, 14, 6571-6603, 10.5194/acp-14-6571-2014, 2014.

Wu, W., Zhao, B., Wang, S., and Hao, J.: Ozone and secondary organic aerosol formation potential from anthropogenic volatile organic compounds emissions in China, J Environ Sci (China), 53, 224-237, 10.1016/j.jes.2016.03.025, 2017.

Zheng, C. H., Shen, J. L., Zhang, Y. X., Huang, W. W., Zhu, X. B., Wu, X. C., Chen, L. H., Gao, X., and Cen, K. F.: Quantitative assessment of industrial VOC emissions in China: Historical trend, spatial distribution, uncertainties, and projection, Atmos Environ, 150, 116-125, 10.1016/j.atmosenv.2016.11.023, 2017.

Zhou, Y., Shuiyuan, C., Lang, J., Chen, D., Zhao, B., Liu, C., Xu, R., and Li, T.: A comprehensive ammonia emission inventory with high-resolution and its evaluation in the Beijing–Tianjin–Hebei (BTH) region, China, Atmos Environ, 106, 305-317, 10.1016/j.atmosenv.2015.01.069, 2015.

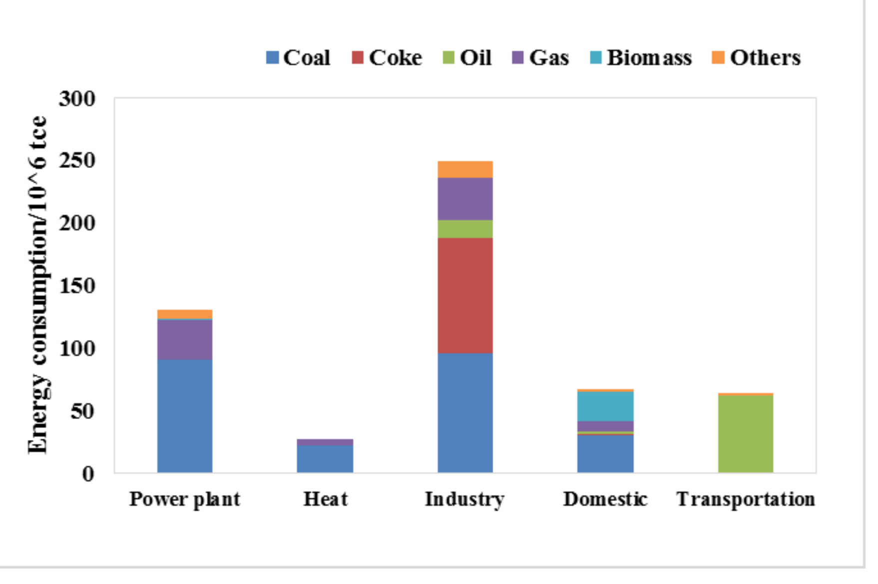


Fig.S1. Energy consumption in Jing-Jin-Ji region in 2014.

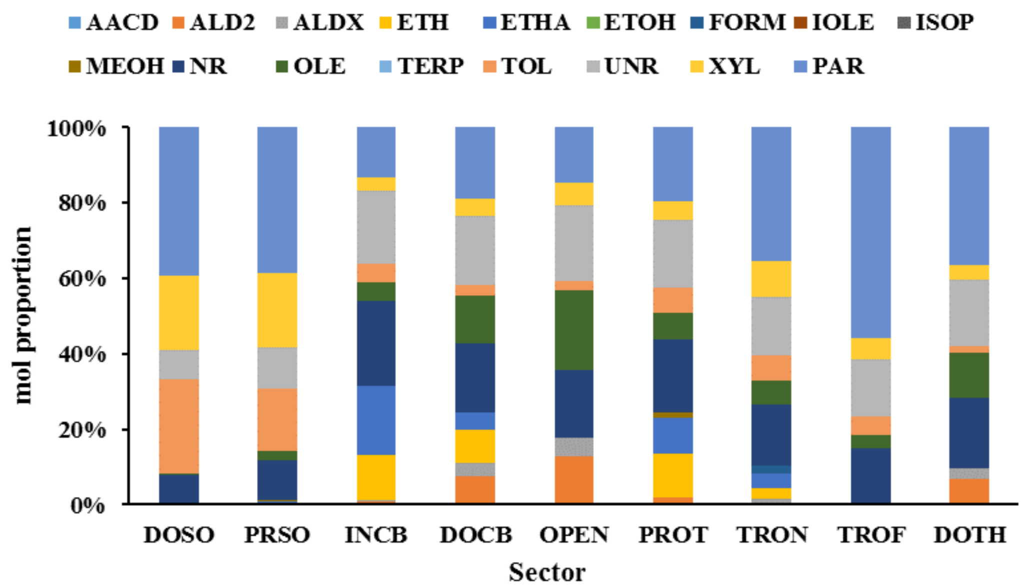
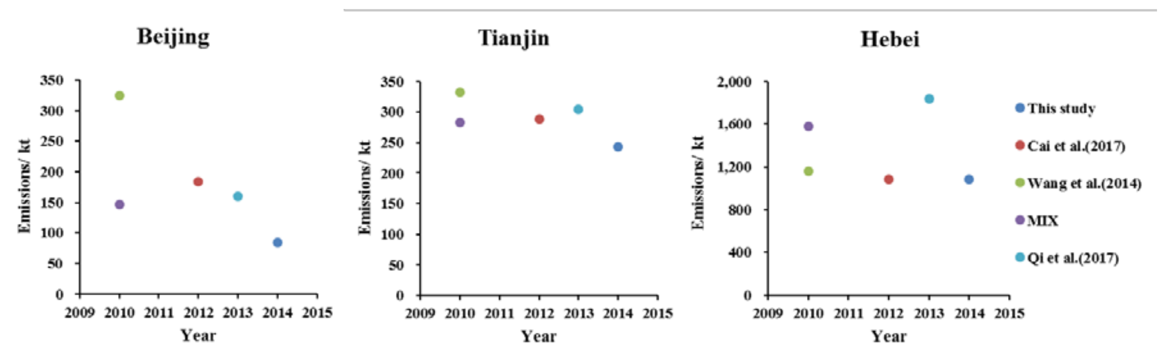
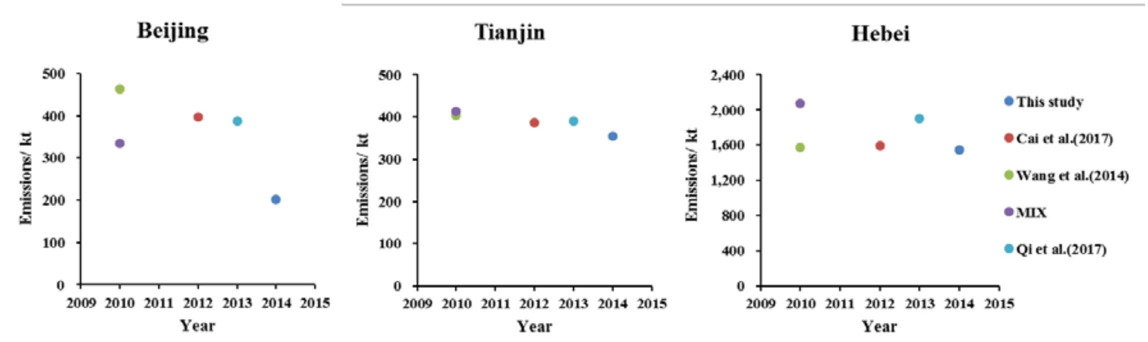


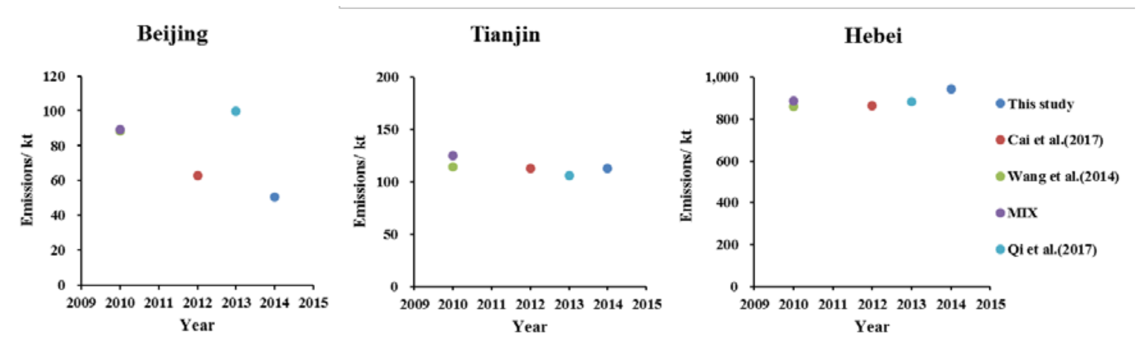
Fig.S2. NMVOCs speciation by sector according to the Carbon Bond 05 (CB05) gas chemistry scheme.



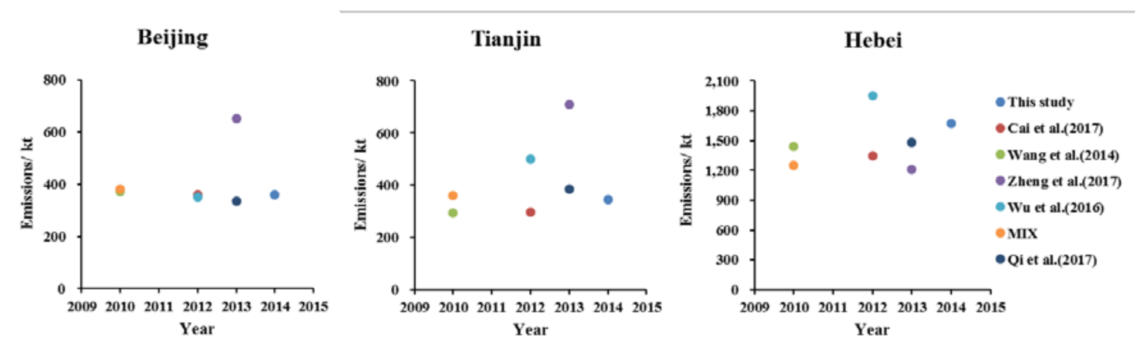
(a)SO_2



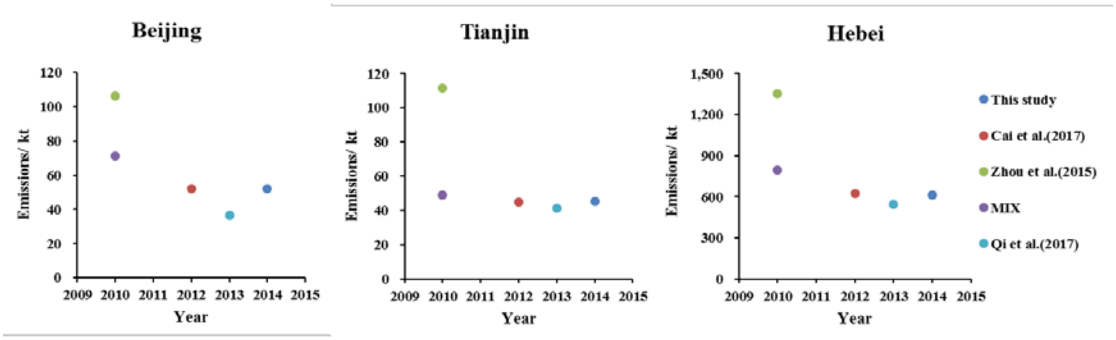
(b)NOx



(c)$PM_{2.5}$



(d)NMVOCs



(e)NH_3

Fig.S3. Emissions compared with other studies.

Table S1 Statistics for validation results of WRF model

Variable	statistics	Unit	January	July	Benchmark
Wind Speed	Mean OBS	m/s	2.68	2.53	
	Mean SIM	m/s	2.65	2.48	
	Mean Bias	m/s	-0.03	-0.05	≤±0.5
	Gross Error	m/s	1.2	1.14	≤2
	RMSE	m/s	1.77	1.56	≤2
	IOA		0.71	0.67	≥ 0.6
Wind Direction	Mean OBS	deg	230.79	205.37	
	Mean SIM	deg	244.79	202.55	
	Mean Bias	deg	3.33	-1.18	≤±10
	Gross Error	deg	41.6	45.93	
Temperature	Mean OBS	K	270.30	298.54	
	Mean SIM	K	269.87	298.77	
	Mean Bias	K	-0.43	0.23	≤±0.5
	Gross Error	K	1.78	2.04	≤2
	RMSE	K	2.28	2.6	
	IOA		0.96	0.94	≥ 0.8
Humidity	Mean OBS	g/kg	1.5	14.0	

Mean SIM	g/kg	1.6	12.9	
Mean Bias	g/kg	0.07	-1.11	≤±1
Gross Error	g/kg	0.31	2.1	≤2
RMSE	g/kg	0.44	2.7	
IOA		0.87	0.8	≥0.6